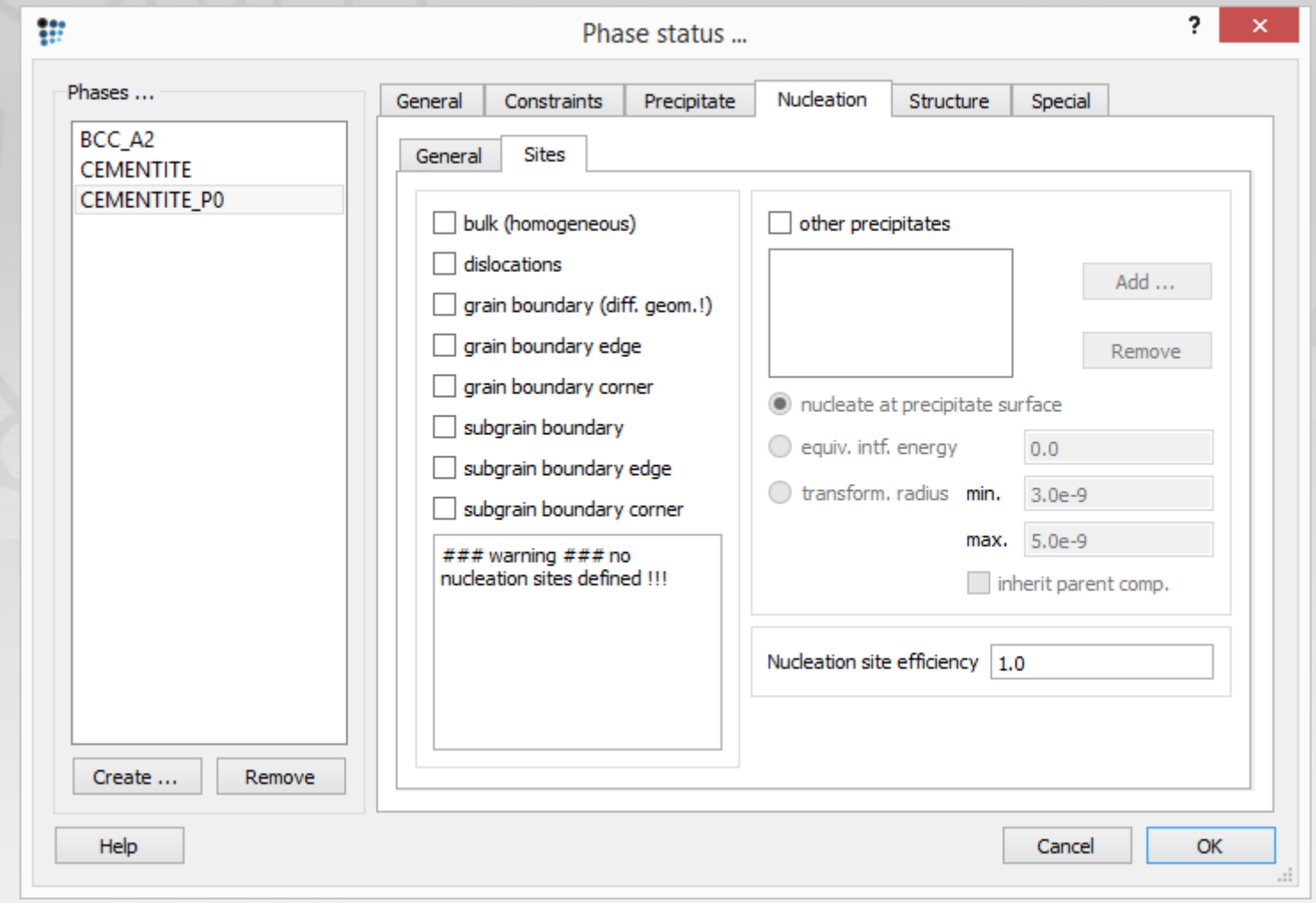
MatCalc
Engineering

MatCalc approach for the modelling of the vacancy concentration evolution

(MatCalc 5.60.0005)

P. Warczok

What is it all about?



What is it all about?

Consequences

- Number of available nucleation sites
- Interfacial energy model
- Precipitate growth & coarsening → nucleation on grain boundaries
- Special cases: Nucleation on/within precipitates

MatCalc Engineering

Number of available nucleation sites

Nucleation rate → $J \sim N_x$

J – Nucleation rate

N_x – Number of nucleation sites on x position

N_A – Avogadro number

V_m – Molar volume

ρ – Dislocation density

Available nucleation sites – bulk

$$N_{bulk} = NA/Vm$$

Available nucleation sites – dislocations

$$N_{disl} = \rho(N_A/V_m)^{1/3}$$

Number of available nucleation sites

Grain&subgrain boundaries – tetra(kai)decahedron concept

Strictly: Truncated octahedron

$$V_{tdh} = 8\sqrt{2}a^3$$

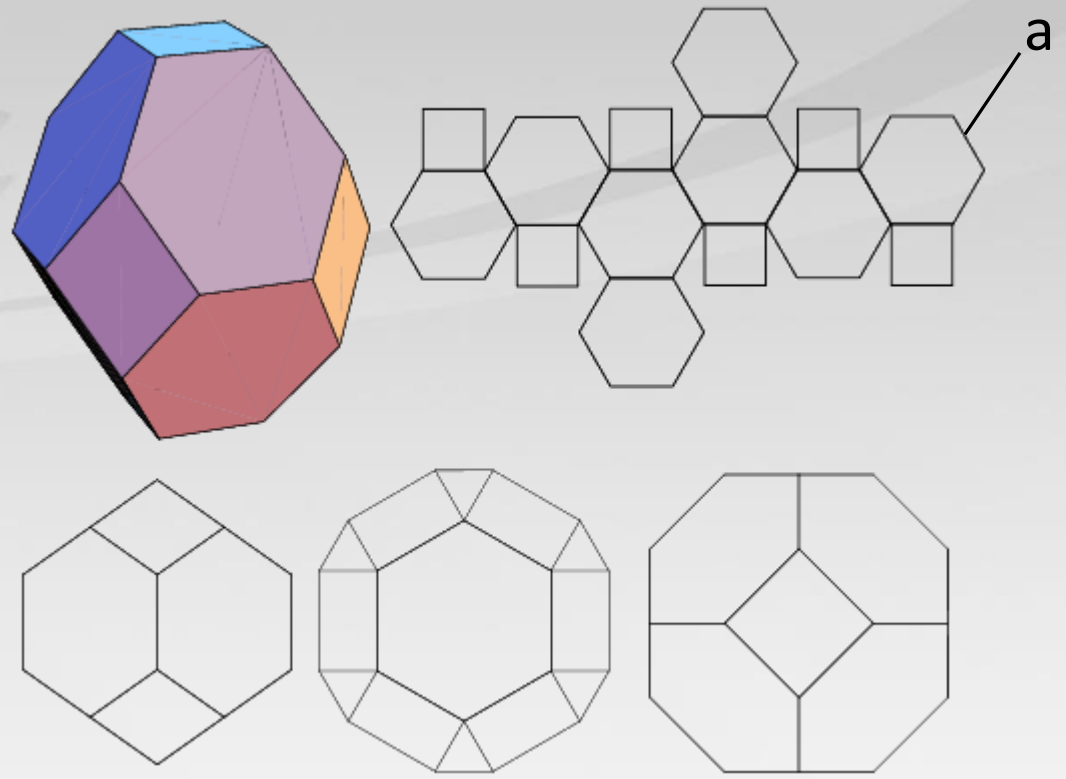
$$S_{tdh} = 6\left(1 + 2\sqrt{3}\right)a^2$$

$$L_{tdh} = 36a$$

V_{tdh} – Volume of the polygon

S_{tdh} – Total surface of the polygon

L_{tdh} – Total edge length of the polygon



http://mathworld.wolfram.com/TruncatedOctahedron.html

Number of available nucleation sites

Grain&subgrain boundaries – tetra(kai)decahedron concept

Strictly: Truncated octahedron

$$V_{tdh} = 8\sqrt{2}a^3$$

$$S_{tdh} = 6\left(1 + 2\sqrt{3}\right)a^2$$

$$L_{tdh} = 36a$$

$$a = \frac{d_{gr/sgr}}{\sqrt{10}}$$

V_{tdh} – Volume of the polygon

S_{tdh} – Total surface of the polygon

L_{tdh} – Total edge length of the polygon

d_{gr} – Grain diameter

d_{sgr} – Subgrain diameter

Number of available nucleation sites

Grain&subgrain boundaries – tetra(kai)decahedron concept

Strictly: Truncated octahedron

$$V_{tdh} = 8\sqrt{2}a^3 + 6a^2H$$

$$S_{tdh} = 6\left(1 + 2\sqrt{3}\right)a^2 + 2a(2H + a)$$

$$L_{tdh} = 36a + 8H$$

$$a = \frac{d_{gr/sgr}}{\sqrt{10}}$$

d_{gr} – Grain diameter

d_{sgr} – Subgrain diameter

D_{gr} – Elongation factor for grains

D_{gr} – Elongation factor for subgrains

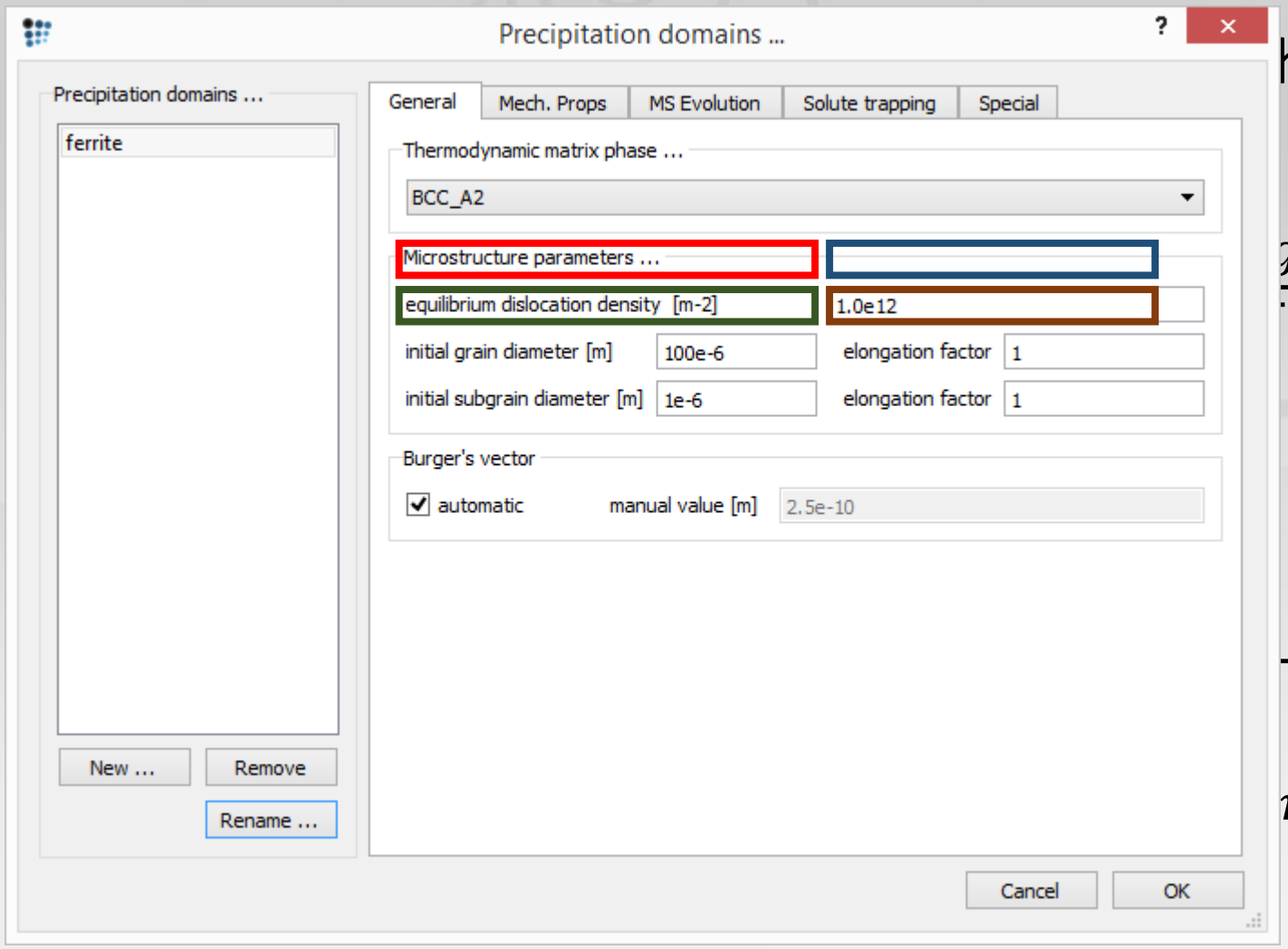
V_{tdh} – Volume of the polygon

S_{tdh} – Total surface of the polygon

L_{tdh} – Total edge length of the polygon

$$H = \sqrt{\left(D_{gr/sgr}^2 - \frac{d_{gr/sgr}^2}{5}\right)} - 2\sqrt{\frac{d_{gr/sgr}^2}{5}}$$

Number of available nucleation sites



hedron concept

gr

d_{gr} – Grain diameter

d_{sgr} – Subgrain diameter

D_{gr} – Elongation factor for grains

D_{gr} – Elongation factor for subgrains

$$r - \frac{d_{gr/sgr}^2}{5}\Bigg) - 2\sqrt{\frac{d_{gr/sgr}^2}{5}}$$

Number of available nucleation sites

Available nucleation sites – grain&subgrain boundaries

$$N_{gb/sgb} = \frac{S_{tdh}}{2V_{tdh}} \left(\frac{N_A}{V_m} \right)^{2/3}$$

Available nucleation sites – grain&subgrain boundary edges

$$N_{gbe/sgbe} = \frac{L_{tdh}}{3V_{tdh}} \left(\frac{N_A}{V_m} \right)^{1/3}$$

Available nucleation sites – grain&subgrain boundary corners

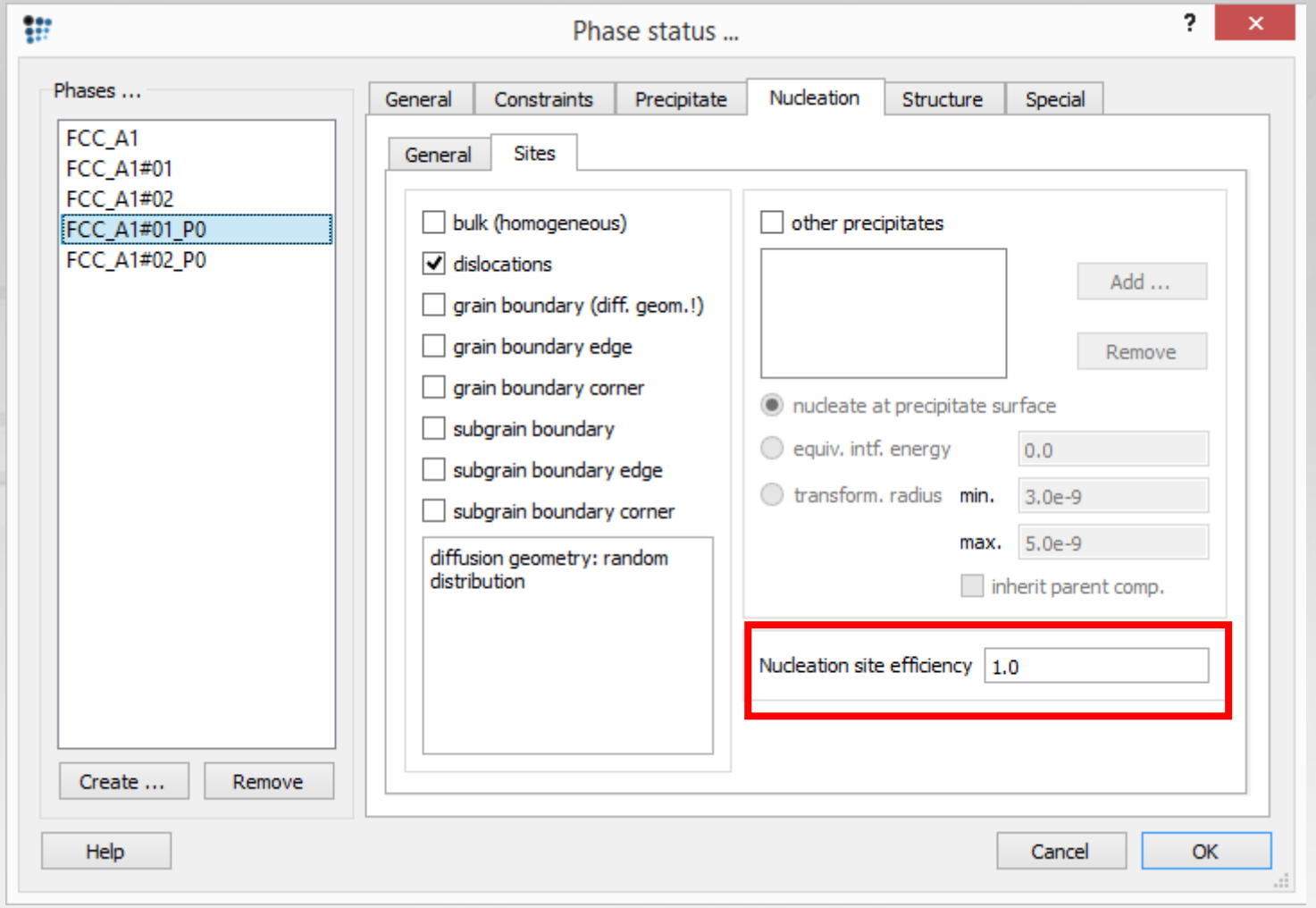
$$N_{gbc/sgbc} = \frac{6}{V_{tdh}}$$

Number of available nucleation sites

„Nucleation site efficiency“

scales linearly the number

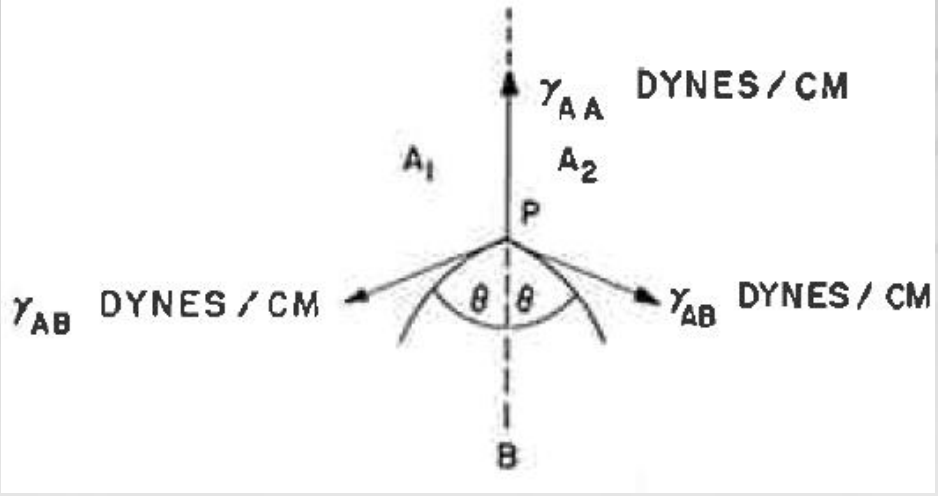
of available nucleation sites



Interfacial energy model

Bulk & dislocations → standard interfacial energy evaluation

Grain & subgrains (surface, edges, corners) → Clemm-Fisher model



$$cos\theta = \frac{\gamma_{AA}}{2\gamma_{AB}}$$

$$a, b, c = \mathrm{f}(cos\theta)$$

γ_{AA} – Grain boundary energy

γ_{AB} – Precipitate/matrix interfacial energy

$$\gamma_{CF} = \frac{(b\gamma_{AB} - a\gamma_{AA})}{\sqrt[3]{36\pi c^2}}$$

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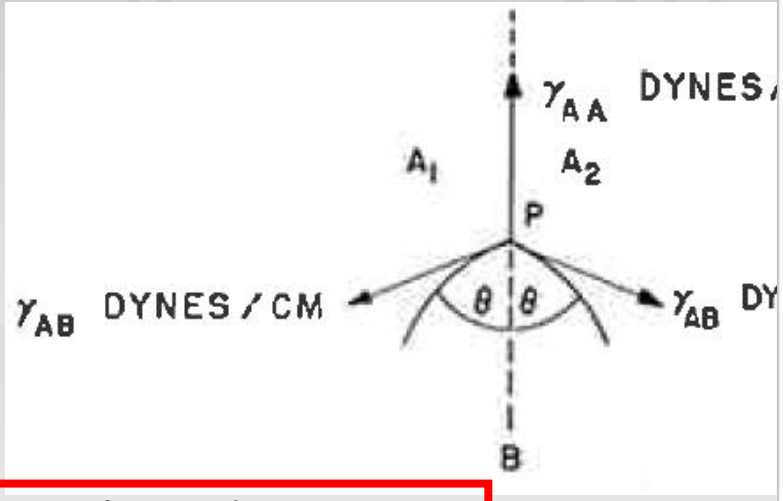
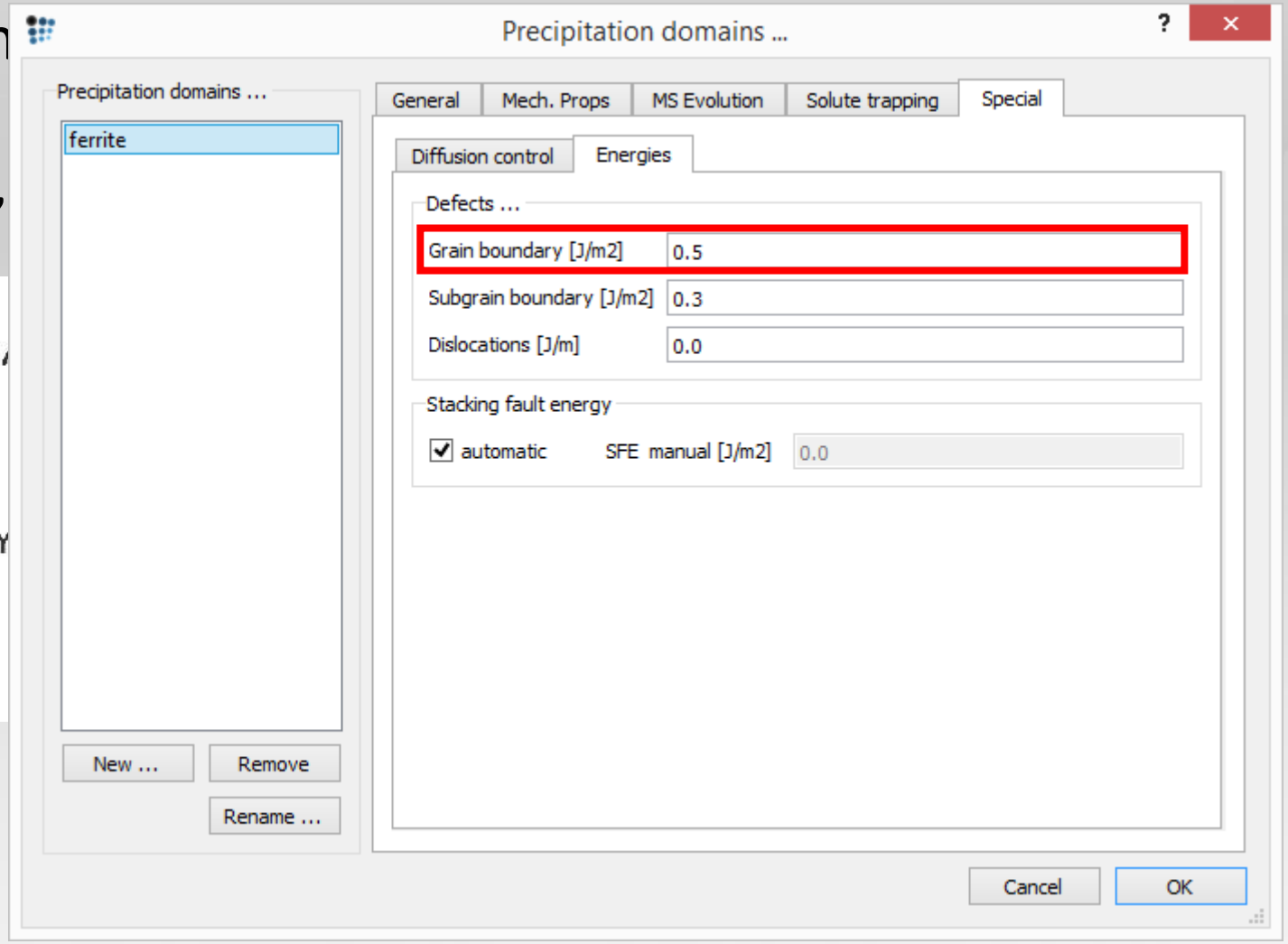
Interfacial energy model

Bulk & dislocations → stan

Grain & subgrains (surface,



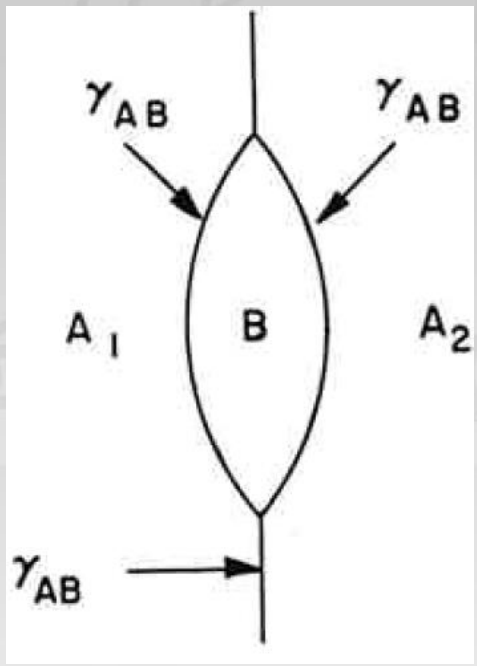


γ_{AA} – Grain boundary energy

γ_{AB} – Precipitate/matrix interfacial energy

Interfacial energy model

Grain & subgrains surfaces



$$a = \pi(1 - cos^2\theta)$$

$$b = 4\pi(1 - cos\theta)$$

$$c = \frac{2}{3}\pi(2 - 3cos\theta + cos^2\theta)$$

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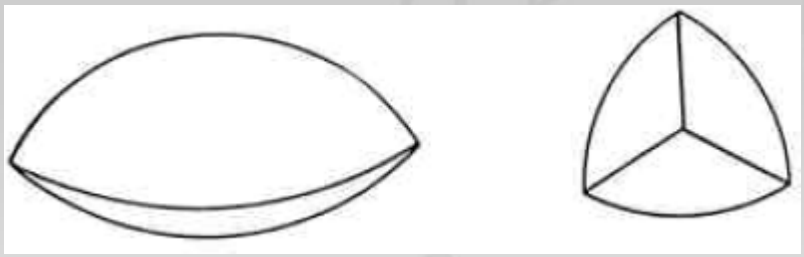
Interfacial energy model

Grain & subgrains edges



$$a = 3\beta(1 - cos^2\theta) - cos\theta\sqrt{(3 - 4cos^2\theta)}$$

$$b = 12\left(\frac{\pi}{2} - \alpha - \beta cos\theta\right)$$

$$c = 2\left(\pi - 2\alpha + cos^2\theta\sqrt{(3 - 4cos^2\theta)} - \beta cos\theta(3 - cos^2\theta)\right)$$

$$\alpha = arcsin\frac{1}{2\sqrt{(1 - cos^2\theta)}}$$

$$\beta = arccos\frac{cos\theta}{\sqrt{3(1 - cos^2\theta)}}$$

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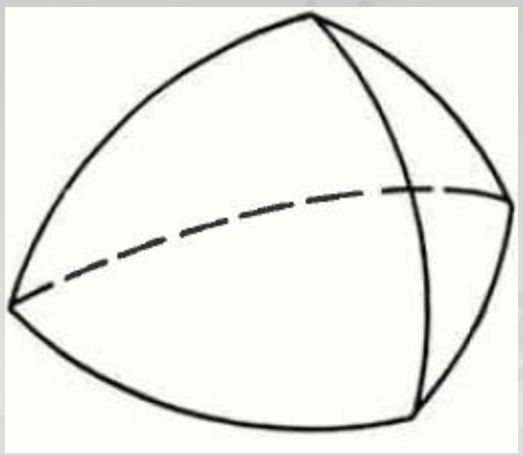
Interfacial energy model

Grain & subgrains corners



$$a = 3\left\{2\phi(1-cos^2\theta) - K\left[\sqrt{1-cos^2\theta-\frac{K^2}{4}}-\frac{K^2}{\sqrt{8}}\right]\right\}$$

$$b = 24\left(\frac{\pi}{3}-\phi cos\theta-\delta\right)$$

$$c = 2\left\{4\left(\frac{\pi}{3}-\delta\right)+Kcos\theta\left[\sqrt{1-cos^2\theta-\frac{K^2}{4}}-\frac{K^2}{\sqrt{8}}\right]-2\phi cos\theta(3-cos^2\theta)\right\}$$

$$K = \frac{4}{3}\sqrt{\left(\frac{3}{2}-2cos^2\theta\right)}-\frac{3}{2}cos\theta \qquad \phi = arcsin\frac{K}{2\sqrt{(1-cos^2\theta)}} \qquad \delta = arccos\frac{\sqrt{2-}cos\theta\sqrt{3-K^2}}{K\sqrt{(1-cos^2\theta)}}$$

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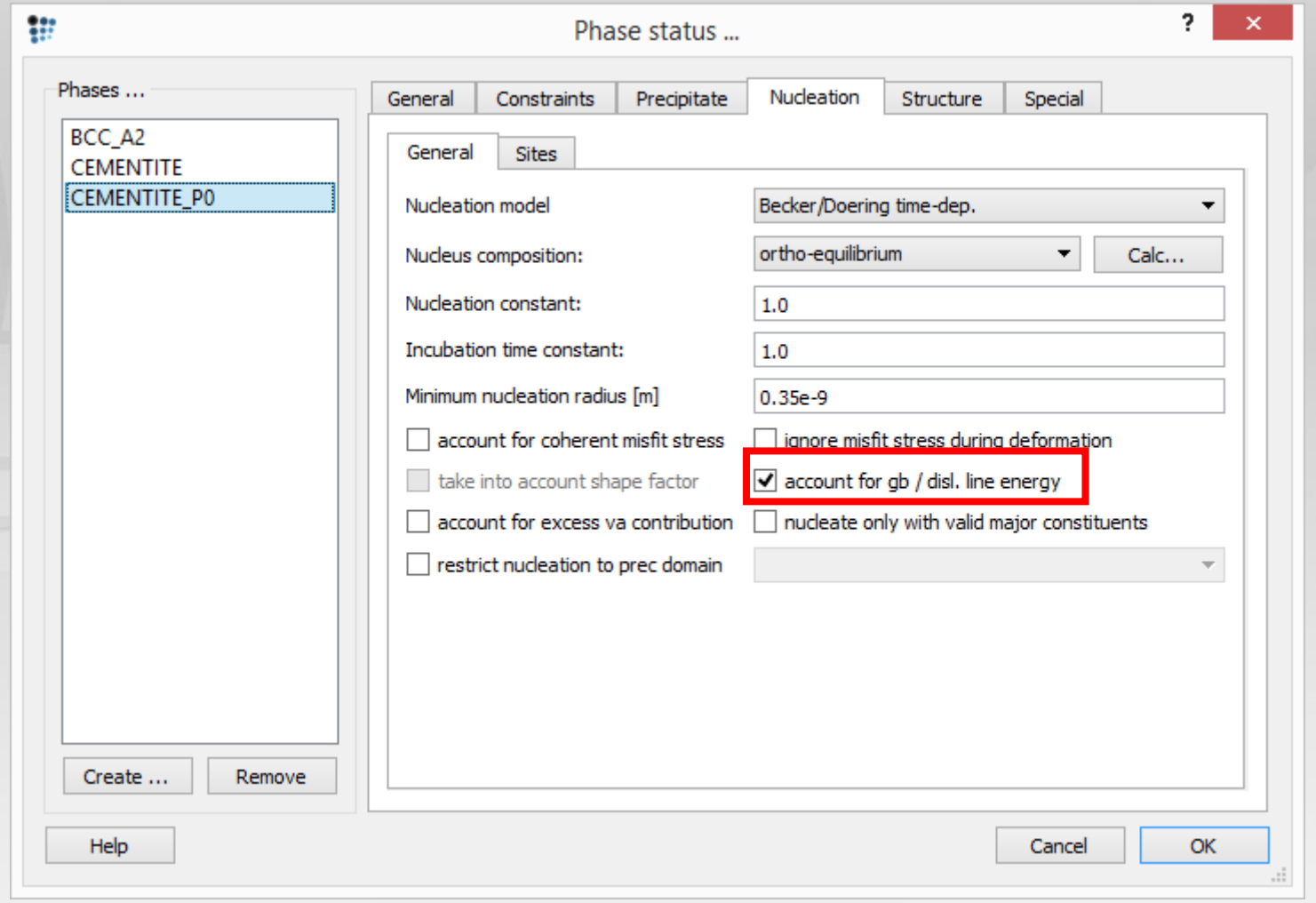
Interfacial energy model

Clemm-Fisher model

needs to be activated!



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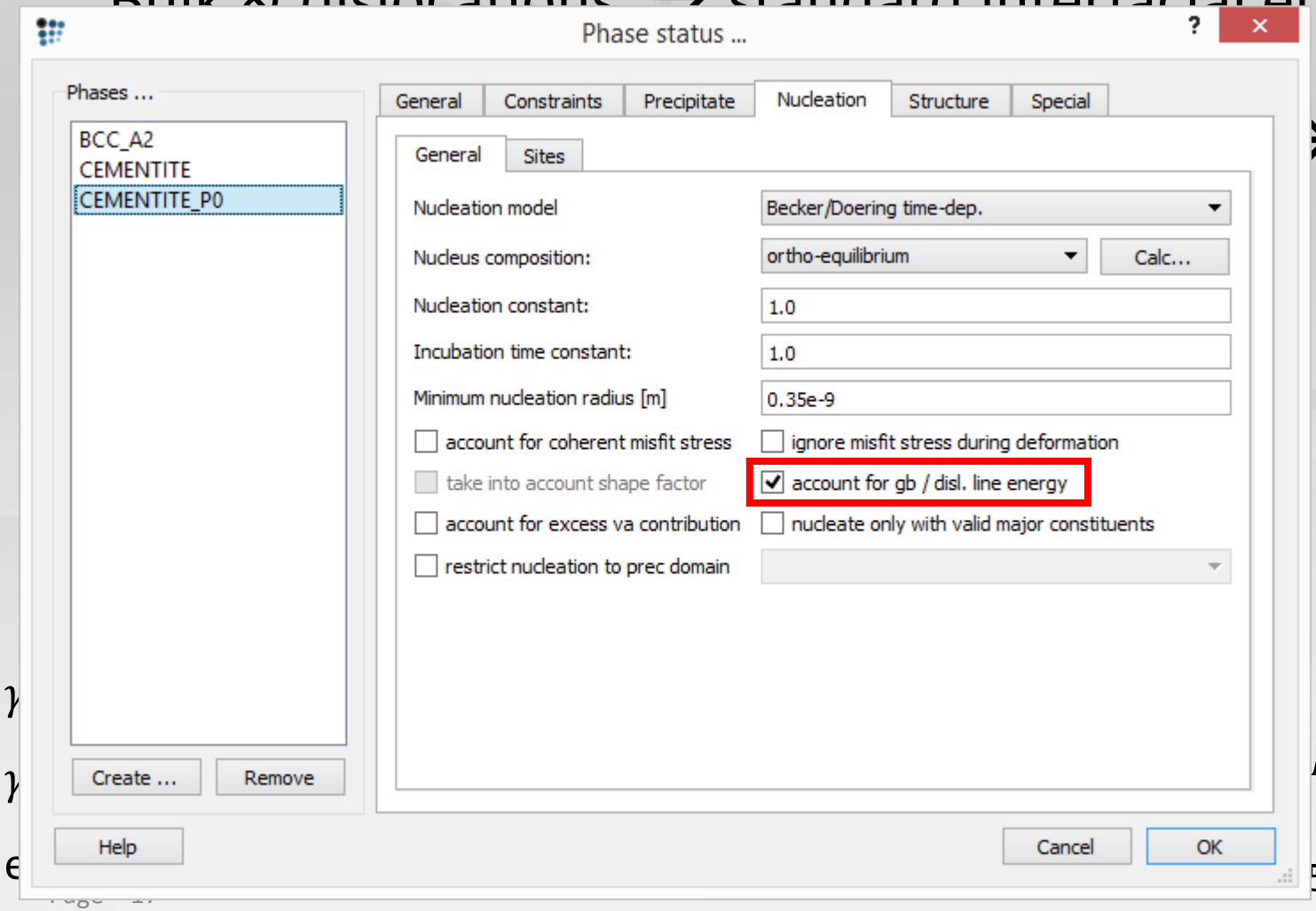
Interfacial energy model

Bulk & dislocations → standard interfacial energy evaluation



→ Clemm-Fisher model

$$cos\theta = \frac{\gamma_{AA}}{2\gamma_{AB}}$$

$$a, b, c = \mathrm{f}(cos\theta)$$

$$F = \frac{(b\gamma_{AB} - a\gamma_{AA})}{\sqrt[3]{36\pi c^2}}$$

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Precipitate growth & coarsening

Difference in diffusion fields

Modelling Simul. Mater. Sci. Eng. **18** (2010) 015011 E Kozeschnik *et al*

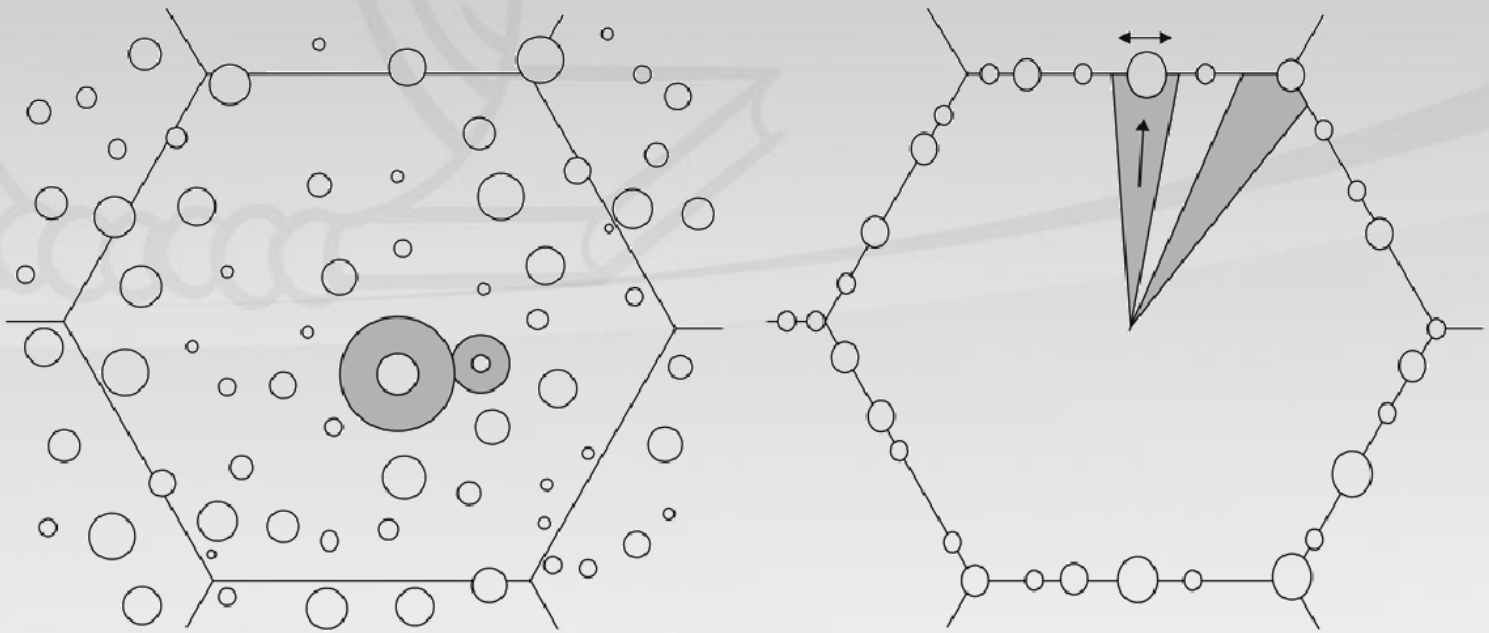
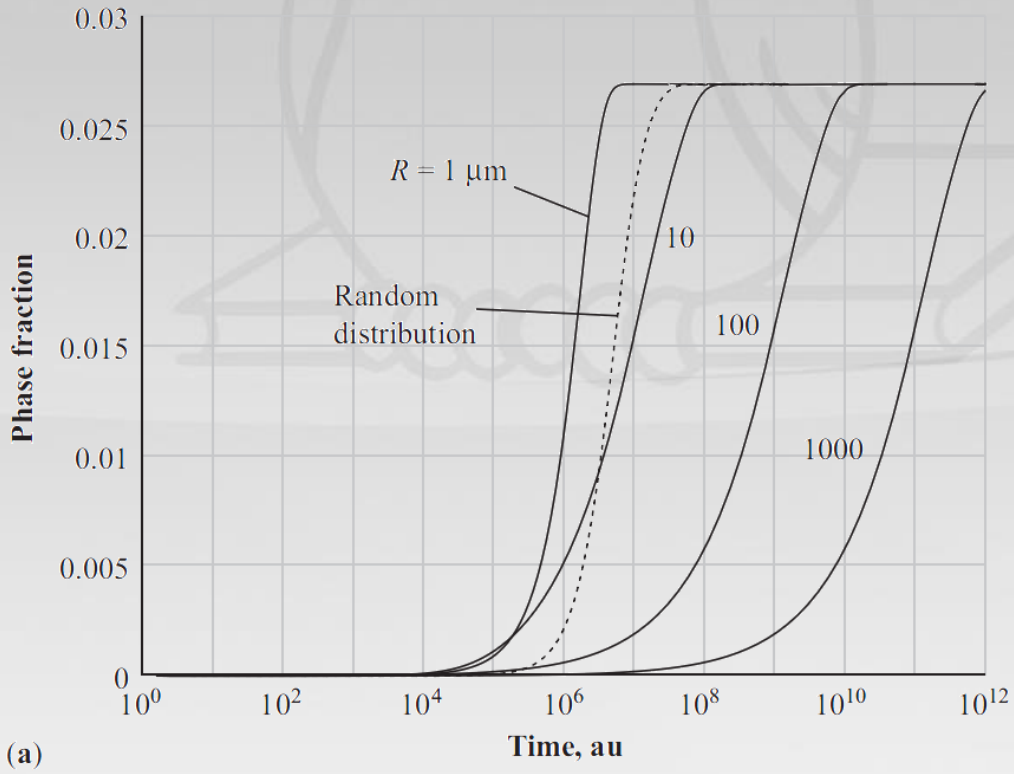
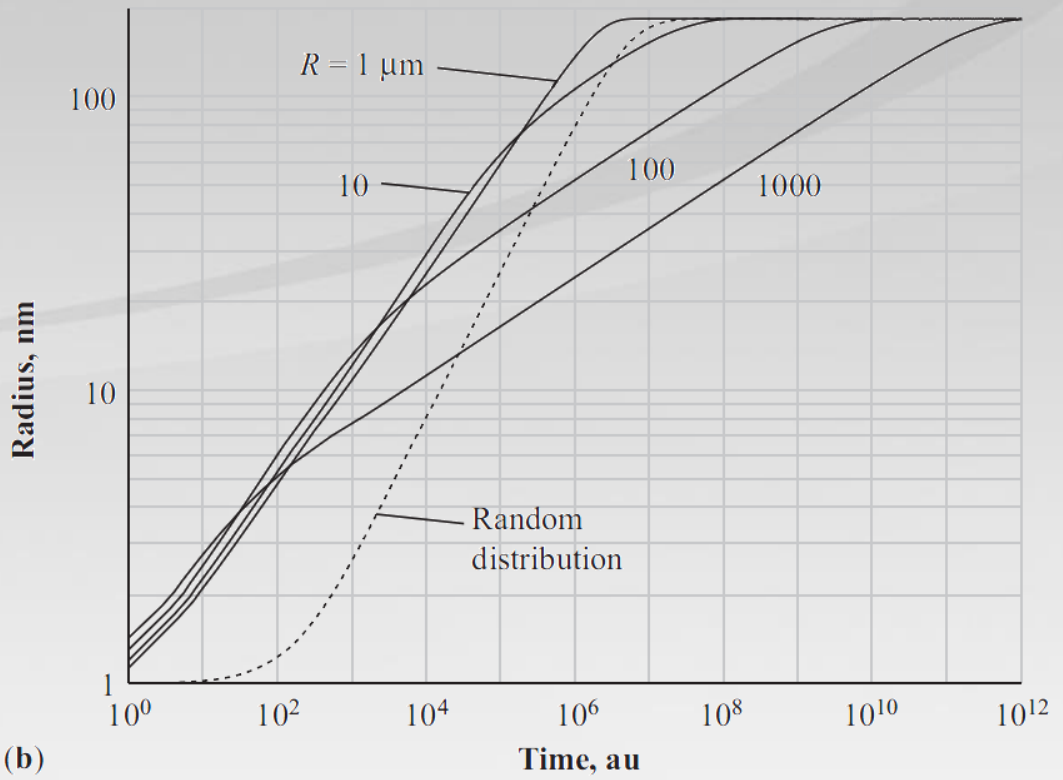


Figure 1. Schematic precipitate distributions and diffusion fields (shaded areas) for random precipitation (left) and heterogeneous precipitation at grain boundaries (right) in 2D.

Precipitate growth & coarsening

Difference in diffusion fields → modification of radius evolution equations derived from thermodynamic extremum principle





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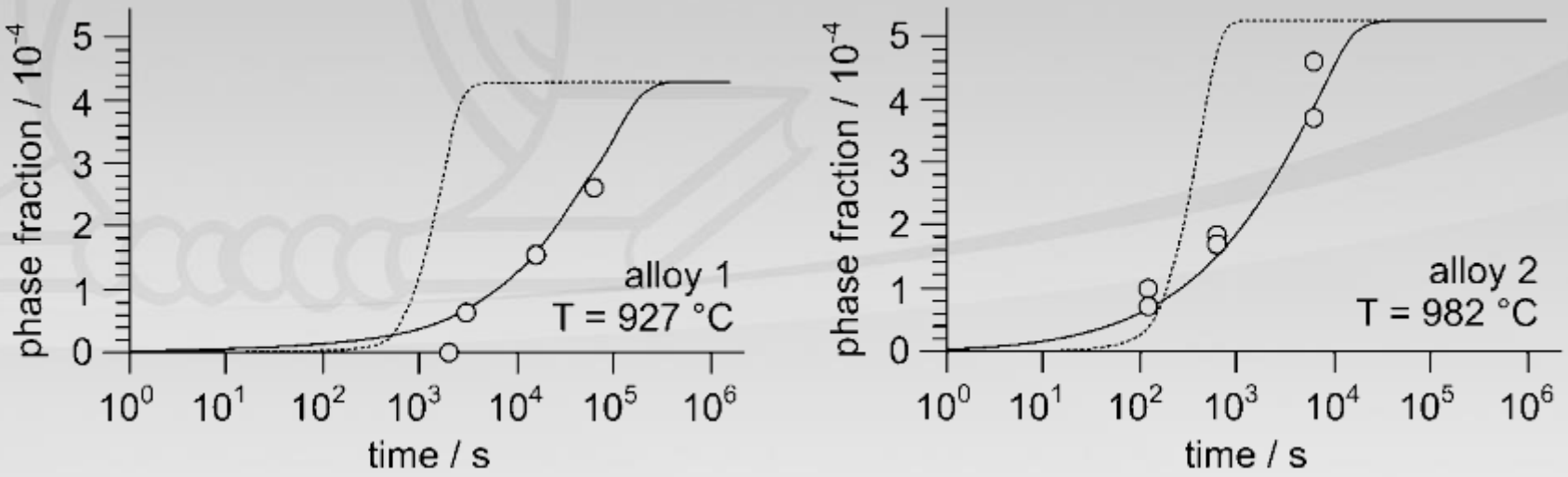
Precipitate growth & coarsening

Difference in diffusion fields → modification of radius evolution equations derived from thermodynamic extremum principle



Precipitation of AlN at austenite at grain boundaries

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Precipitate growth & coarsening

Differ
eq

NOTE:

- The grain boundary diffusion field model is automatically used when "grain boundary" is selected as the nucleation site
- This model is relevant for the system with large grain size and small precipitate phase fractions.
- In other cases, use the random diffusion field model → select other nucleation sites (e.g. "dislocations") and adjust the available number of the nucleation sites using the "nucleation site efficiency"

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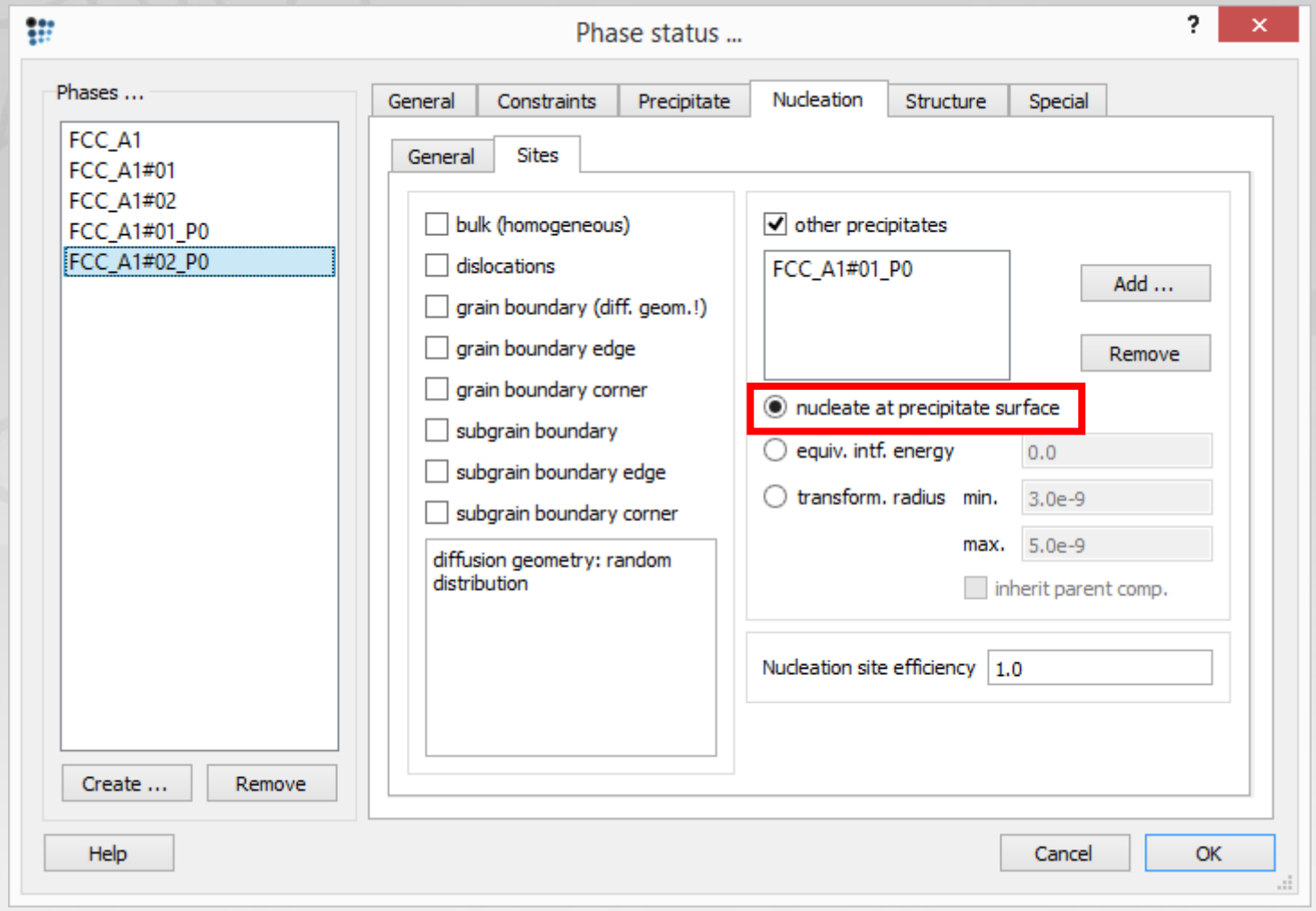
Nucleation on the precipitate surface



Nucleation on the precipitate surface

Available nucleation sites → atoms on the surface of the parent phase

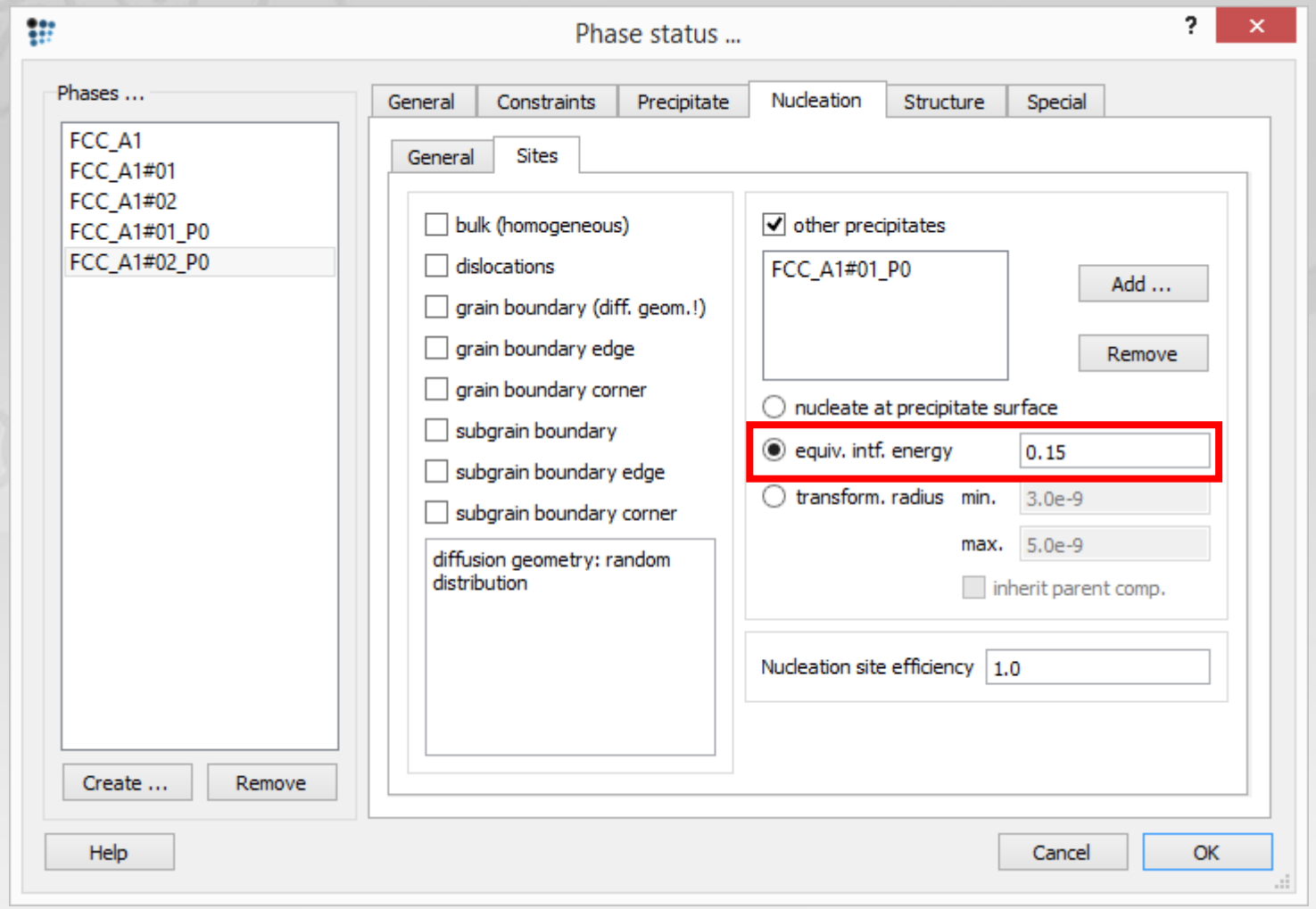
$$N_{prec,surf} = 4\pi \left(\frac{N_A}{V_m}\right)^{2/3} \left(\sum_{class} N_j r_j^2\right)$$

N_j - Number of precipitates in class „j“

r_j - Radius of precipitates in class „j“

Parent phase is not modified by the nucleation of the new phase

Nucleation within the precipitate



Nucleation within the precipitate

Available nucleation sites → atoms on the surface of the parent phase (as in the previous case)

Nucleation → $d_{new} > d_{parent}$ $d_{nucl,new} = d_{new} - d_{parent}$

d_{new} - Driving force of the new phase

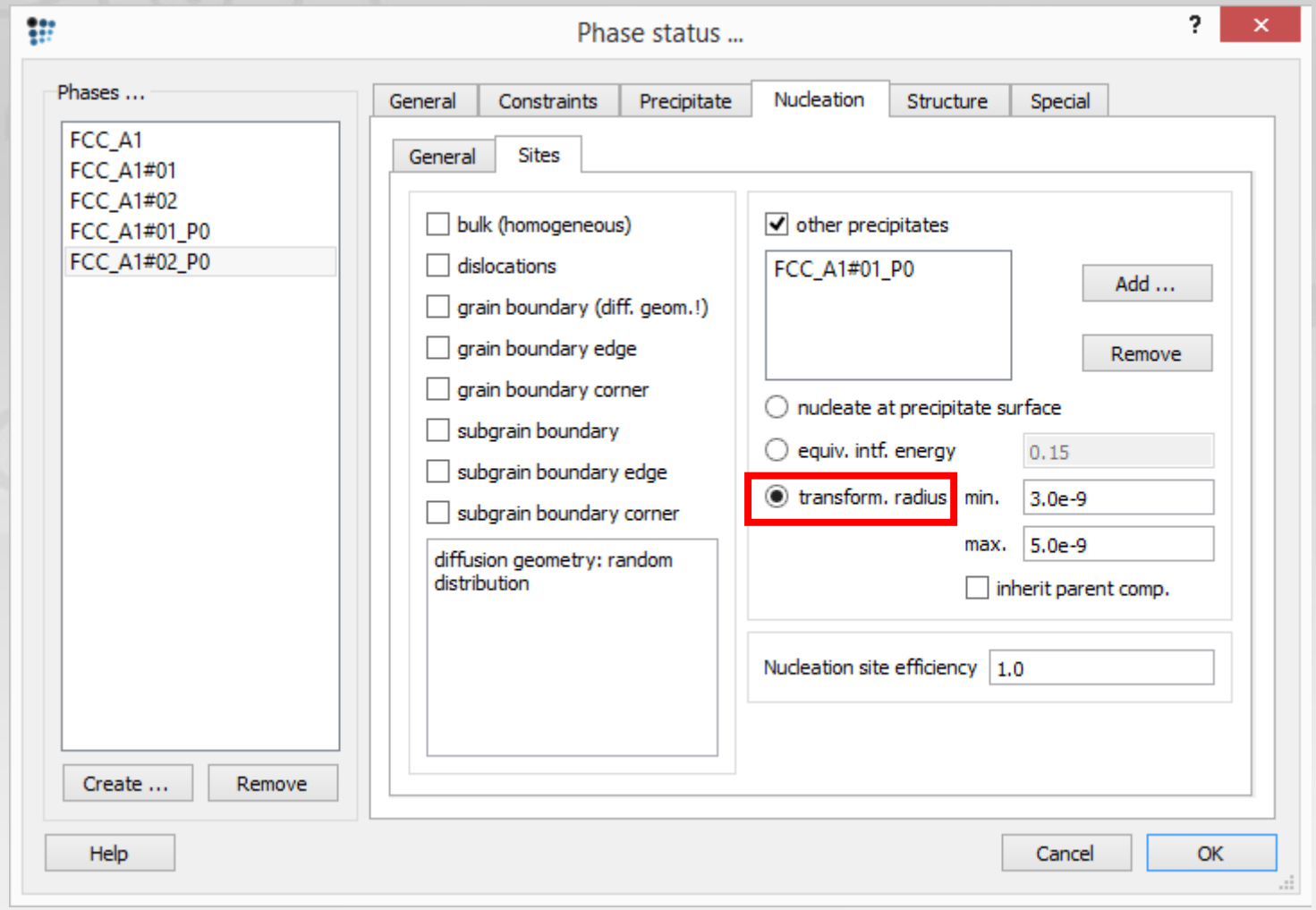
d_{parent} - Driving force of the parent phase

$d_{nucl,new}$ - Nucleation driving force of the new phase

Interfacial energy defined by user, critical radius from parent prec.

Parent phase transforms gradually into the new one

Transformation of the precipitate



Transformation of the precipitate

„Transformation towards“ rather than „nucleation of“ the new precipitate

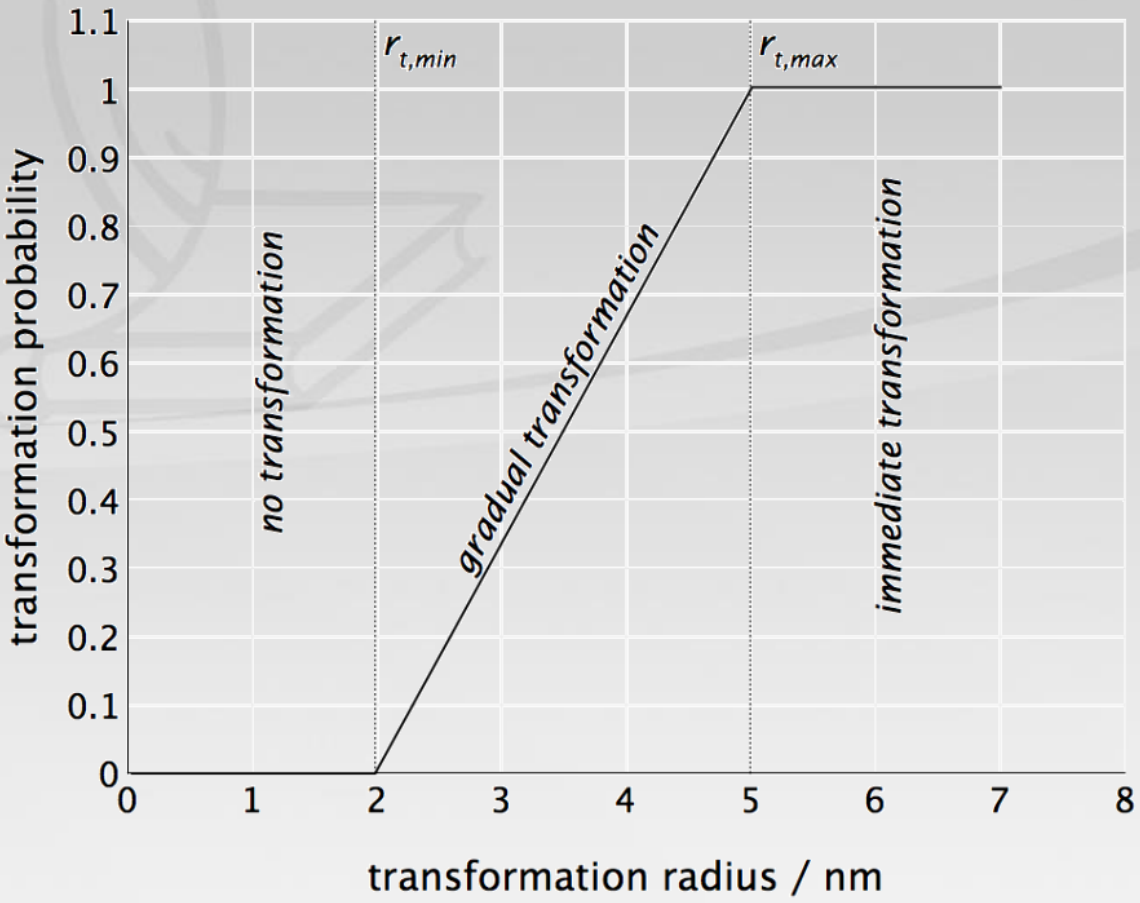
Transformation condition: $d_{new} > d_{parent}$, $d_{nucl,new} = d_{new} - d_{parent}$

New precipitate size taken from the parent phase

Initial precipitate composition might be taken from the parent phase

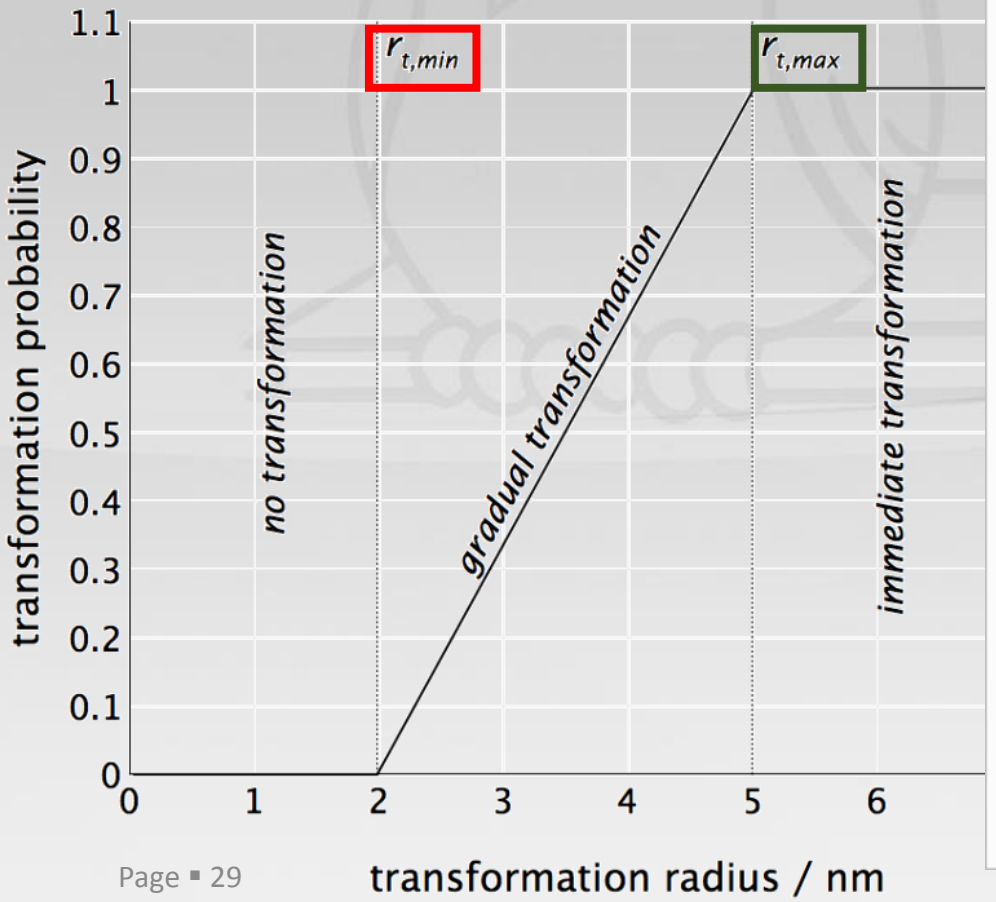
Transformation of the precipitate

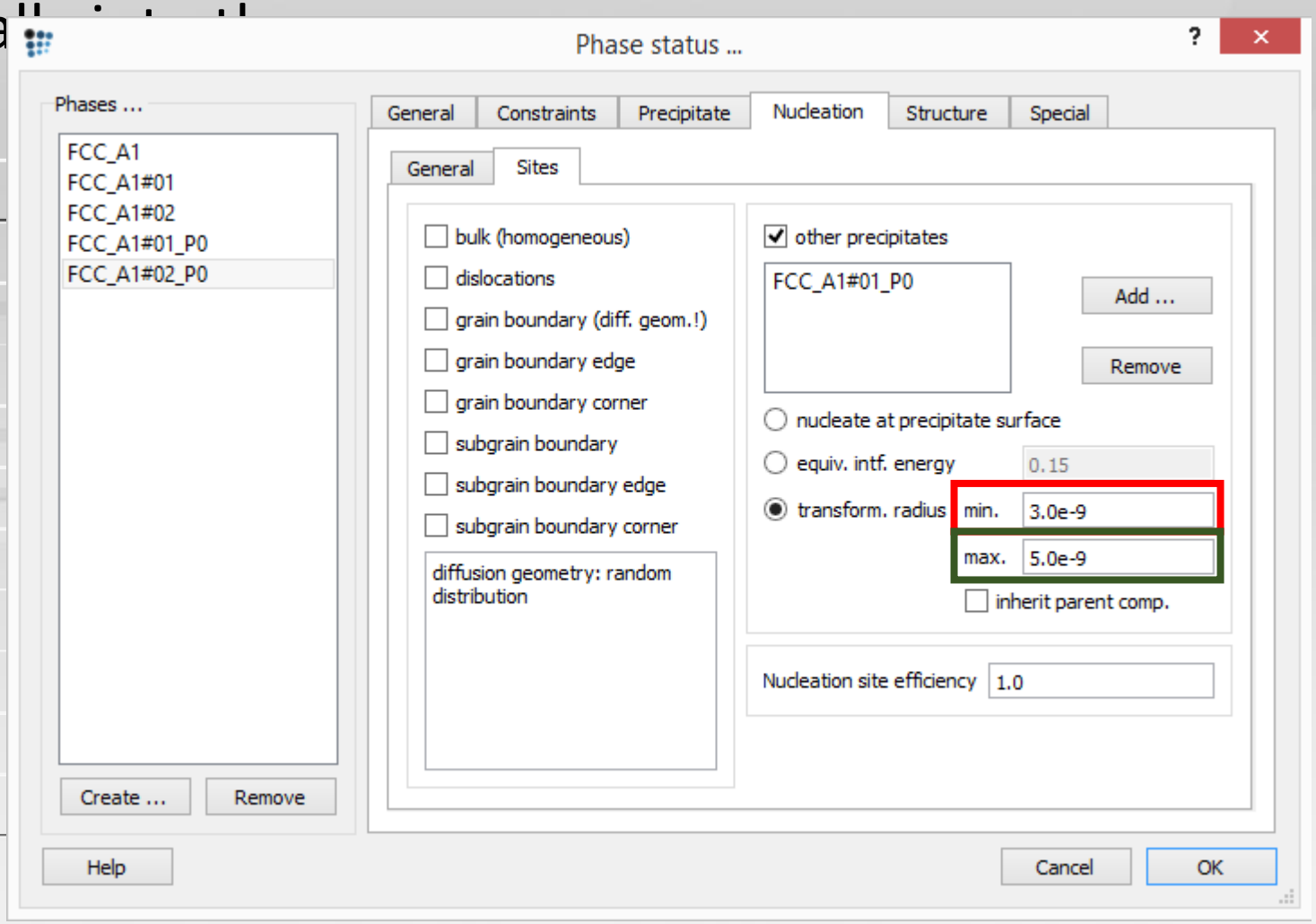
Parent phase transforms gradually into the new one



Transformation of the precipitate

Parent phase transforms gradua

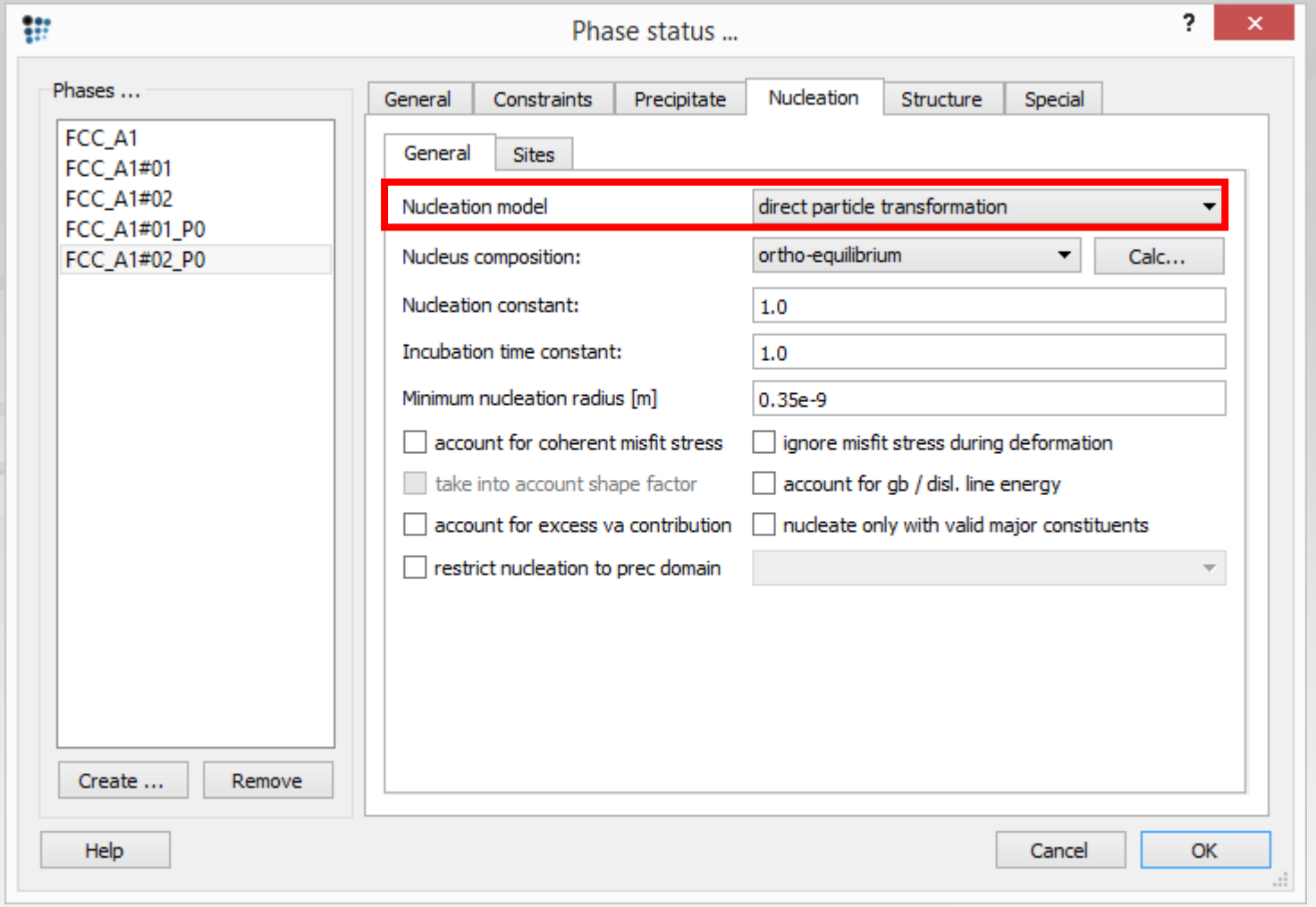




Direct particle transformation

For the two last cases:
(nucleation within and transformation of the precipitate)

Change the nucleation model to „direct particle transformation“!



Acknowledgments

- Yao Shan